Degeneracy and Consistency Condition of Berry phases:
Gap Closing under the Twist

T. Hirano,[1, *] H. Katsura,[1, †] and Y. Hatsugai[1, 2, ‡]

^{1}*Department of Applied Physics, The University of Tokyo,*
7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan
^{2}*Institute of Physics, University of Tsukuba, 1-1-1 Tennodai, Tsukuba, Ibaraki 305-8571, Japan*
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We have discussed a consistency condition of Berry phases defined by a local gauge twist and spatial symmetries of the many body system. It imposes a non trivial gap closing condition under the gauge twist in both finite- and infinite-size systems. It also implies a necessary condition for the gapped and unique ground state. As for the simplest case, it predicts an inevitable gap closing in the Heisenberg chain of half integer spins. Its relation to the Lieb-Schultz-Mattis theorem is discussed based on the symmetries of the twisted Hamiltonian. The discussion is also extended to the (approximately) degenerated multiplet and fermion cases. It restricts the number of the states in the low energy cluster of the spectrum by the filling of the fermions. Constraints by the reflection symmetry are also discussed.

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For the last decade, quantum criticality with gapless excitations have been focused in its relation to a quantum phase transition. Generically speaking, the gapless phase is only realized by a fine tuning of the parameters of the quantum hamiltonian. Some machinery to protect the gap closing of the quantum mechanical system is necessary. Symmetries as a spatial translation can be one of the reasons which plays an important role in the Fermi liquids. Today we have other several machinery for the gap closing in a generic situation. One is the Nambu-Goldstone mechanism. When a continuous symmetry is broken spontaneously, there can be a gapless excitation by slowly varying its local order parameter which is responsible for the symmetry breaking. It is closely related to the Lieb-Schultz-Mattis(LSM) argument[1, 2, 3, 4, 5, 6, 7] to prove existence of the gapless excitations in a half-odd-integer spin chains. This LSM argument is justified in restricted situations. It allows existence of a gapped phase which is known as the Haldane phase in the integer spin chains. This is a typical quantum liquid where strong quantum fluctuations prevent from forming an ordered phase. The other mechanism to protect the gapless excitations is an appearance of the edge states such as the one in quantum Hall states and Haldane phases[8, 9, 10, 11, 12, 13, 14, 15, 16]. There is a fundamental class of physical phases with intrinsic energy gap as topological insulators. They are gapped quantum liquids in a bulk without any fundamental symmetry breaking. However the system has a geometrical (topological) perturbation such as the existence of the boundaries, low energy modes (quasi-particle) as the generic edge states appear and the phase becomes gapless when the boundaries are infinitely separated.

The existence of the energy gap is also closely related to the degeneracy of the ground state. When the discrete symmetry is broken such as for the Heisenberg spins with ising anisotropy or charge ordered states, the symmetry broken states split into a low energy cluster with small energy splitting in a finite periodic system. The exact degeneracy is only realized in the infinite size limit. For the topological insulators without any symmetry breaking, there can be additional degeneracy as the topological degeneracy which characterizes the non trivial quantum liquids[17, 18].

As for the topological insulators, quantum order parameters by the many body Berry phases, associated with the local gauge twists, have been proposed and its validity is justified for several concrete models [19, 20, 21]. Using this Berry phase and its symmetry property, we prove that there is an inevitable degeneracy during the twist as for some classes of Hamiltonian which is also related to the LSM theorem. Our discussions are valid not only in infinite-size systems but also in finite-size systems, which can be applicable for various correlated electron systems.

Let us define a local order parameter γ_{ij} at a link (ij) by the Berry phase[22] $i\gamma_{ij} = \int_0^{2\pi} d\phi A_{ij}(\phi)$, where $A_{ij}(\phi)$ is a Berry connection obtained from a gauge fixed (single valued) normalized ground state $|\psi_{ij}\rangle$ of a Hamiltonian $H_{ij}(\phi)$ as $A_{ij}(\phi) = \langle\psi_{ij}|\partial_\phi|\psi_{ij}\rangle$ [19], where ϕ is a parameter of the local $U(1)$ twist on the link. It is gauge dependent but is well defined up to modulo 2π. Further it is quantized if the ground state is invariant under some anti-unitary operation. As for the Heisenberg model with generic connectivity, the Hamiltonian with the local twist is given as $H_{ij}(\phi) = J_{ij}\left((e^{i\phi}S_i^+ S_j^- + e^{-i\phi}S_i^- S_j^+)/2 + S_i^z S_j^z\right) + \sum_{(kl)\neq(ij)} J_{kl}\boldsymbol{S}_k \cdot \boldsymbol{S}_l$. We should note that the Berry phase is only well defined unless the energy gap between the ground state and the first excited states does not vanish during the twist.

Since the twist on the the link can be modified by the local gauge transformation, it gives some constraints

for the Berry phase distribution. For simplicity, let us first discuss the one dimensional nearest neighbor antiferromagnetic Heisenberg model of generic spins on a finite lattice. We discuss within the subspace of fixed $S^z_{tot} = \sum S^z_j$ since it commutes with $H_{i,j}(\phi)$. Performing a local gauge transformation at the site j as

$$U_j(\phi) = e^{i(S - S^z_j)\phi}, \quad \phi \in [0, 2\pi]$$

which is single valued in the parameter space, one has an important relation between the two different hamiltonians (which are gauge equivalent), $H_{j,j+1}$ and $H_{j-1,j}$ as $H_{j,j+1} = U^\dagger_j H_{j-1,j} U_j$. Correspondingly the states are mapped into each other as $|\psi_{j,j+1}\rangle = U^\dagger_j|\psi_{j-1,j}\rangle$, where $|\psi_{j-1,j}\rangle$ and $|\psi_{j,j+1}\rangle$ are two different ground states of $H_{j-1,j}$ and $H_{j,j+1}$, respectively. Note that, if the state $|\psi_{j-1,j}\rangle$ is gauge fixed as a single valued in the parameter space, it is also true for the state $|\psi_{j,j+1}\rangle$. Assuming that *the ground state is unique and gapped during the twisting*, this simple relation gives a constraint for the quantum local order parameters γ_{ij}'s

$$
\begin{aligned}
\gamma_{j,j+1} &= -i \int \langle \psi_{j-1,j} | U_j \partial_\phi (U^\dagger_j | \psi_{j-1,j}\rangle) \, d\phi, \\
&= \gamma_{j-1,j} + \int (S - \langle \psi | S^z_j | \psi \rangle) \, d\phi.
\end{aligned}
$$

Since the expectation value of the hermitian operator S^z_j is independent of the gauge transformation, we have dropped the label of the wave function to specify the position of the twist. The time reversal invariance of the state $|\psi\rangle$ implies $\langle \psi | S^z_i | \psi \rangle = -(\langle \psi | S^z_i | \psi \rangle)^* = 0$. Then, one obtains

$$\gamma_{j-1,j} = 2\pi S + \gamma_{j,j+1}.$$

Since the present 1D Heisenberg model has a translational symmetry, the Berry phases as the quantum order parameters should also respect this translational symmetry, that is, γ_{ij} should be independent of the link (ij) in mod 2π unless they are well defined. However this is impossible for the half integer spins due to the above constraint $\gamma_{j-1,j} \equiv \gamma_{j,j+1} + \pi$, (mod$2\pi$). It implies that *there is a gap closing under the local twist, as for the antiferromagnetic Heisenberg chains with half-integer spins on a finite lattice.* Although our results can be applicable for arbitrary half integer spins, similar conclusions for the $S = 1/2$ case are also obtained from different analysis [7, 23, 24]. As for the integer spin Heisenberg model, the above constraint does not forbid uniform distribution of the Berry phase γ_{ij}. Actually the uniform π Berry phase is realized in a $S = 1$ case[19, 21, 25].

The idea here is extended to the general cases without any difficulty. Let us consider sets of some generic twists for several links labeled by "In". Assuming the uniqueness of the ground state even under the twisting, one can define the Berry phase γ_{In}. Next let us perform a set of
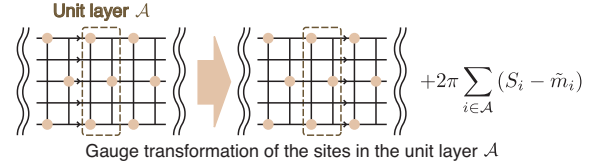

FIG. 1: The definition of the unit layer, and the gauge transformation of the Berry phase. The arrows on links denotes the link twist.

the local gauge transformation within the area $\mathcal{A}$. Then we have a new set of twists labeled by "Out". Under this generic setup, one has a constraint between the two corresponding Berry phases γ_{In} and γ_{Out} as

$$\gamma_{\text{In}} = \gamma_{\text{Out}} + 2\pi \sum_{i \in \mathcal{A}} (S_i - \tilde{m}_i), \quad \tilde{m}_i = \frac{1}{2\pi} \int \langle \psi | S^z_i | \psi \rangle d\phi.$$

Translational symmetry For a spin ladder as an example of translational invariant case, we take $\mathcal{A}$ as a unit layer and define Berry phase by twisting the links on the left boundary of the area $\mathcal{A}$ simultaneously (see FIG.1). Due to the translational symmetry, we have a constraint for the Berry phases as $\gamma_{\text{In}} \equiv \gamma_{\text{Out}}$ (mod 2π) assuming that the ground state is gapped under the twisting. Since the total S^z is conserved, we have $\sum_{i \in \mathcal{A}} \tilde{m}_i = (1/2\pi) \int d\phi \langle \psi | \sum_i S^z_i | \psi \rangle / N = \langle \psi | \sum_i S^z_i | \psi \rangle / N = |\mathcal{A}| m$, where $|\mathcal{A}|$ is a number of sites in the unit layer and m is the average magnetization (N is a number of the unit layers). Note that the translational invariance of the magnetization at arbitrary ϕ is guaranteed by the fact that S^z_{total} commutes with a unitary transformation which spreads the flux in a transitionally invariant way. Then we have a necessary condition for the unique and gapped ground state as

$$\sum_{i \in \mathcal{A}} (S_i - m) \equiv \nu \in \mathbb{Z}$$

It is a condition to have a magnetization plateau[26].

By considering a non-Abelian Berry phase[19], this argument can be extended to the case with (approximate) degeneracy. Now let us assume the low energy spectrum near the ground states forms a multiplet $\Psi = (|\psi_1\rangle, \cdots, |\psi_M\rangle)$ with M eigenstates, $|\psi_i\rangle$ ($i = 1, \cdots, M$). Here, we assume that they are in the subspace of the same S^z_{tot} and the energy gap above the multiplet is stable. Then as for the Berry phase $\gamma = \int d\phi \, \text{Tr} \, \Psi^\dagger \partial_\phi \Psi$, we have a relation $\gamma_{\text{In}} = \gamma_{\text{Out}} + 2\pi M \nu$ based on the same assumption. Therefore as for the translational invariant system, we have a consistency requirement $2\pi M \nu \equiv 0$ (mod 2π) assuming the gap even under the twist. Then *as for $\nu = \sum_{i \in \mathcal{A}} (S_i - m) = \frac{p}{q}$ with mutually co-prime p and q case, M has to be a multiple of q, that is, the low energy spectrum has to form a cluster of $q\ell$ states (ℓ: integer).* This situation naturally occurs with discrete symmetry breaking [27] or topological degeneracy.

As for the $S = 1/2$ Heisenberg ladder with n legs, the discussion here predicts a gap closing under the twist when n is odd[28, 29]. It allows to have an energy gap above the low energy multiplet composed of two states even with the $S = 1/2$ system, which is realized for the spin tube[30]. The present argument also gives a consistent description for ferrimagnets discussed by the effective field theory and the LSM argument[31]. Consider a Heisenberg spin chain with different spin quantum numbers as $S_j = S_1$ for $j = 1 \pmod{M}$ and $S_j = S_2$ for others. Taking the unit layer to include these M spins, the gauge transformation yields the relation of the Berry phase as $\gamma_1 = \gamma_2 + 2\pi(S_1 + (M-1)S_2)$. The system must have the gapless excitations or the ground state degeneracy if $(S_1 + (M-1)S_2) \notin \mathbb{Z}$, and the system can have a unique and gapped ground state if $(S_1 + (M-1)S_2) \in \mathbb{Z}$.

We shall now discuss the connection to the LSM theorem. Our argument suggests that there is at least one level-crossing point during the local twist if Berry phases cannot be arranged in a compatible way with the translational symmetry. Indeed, one can rigorously show the degeneracy of the ground state at $\phi = \pi$. For simplicity, we consider the first example, namely the half-integer Heisenberg spin chain with length L in a zero magnetic field. We introduce the following two symmetry operations. One is $U_j(\phi)T$, where T is the operation for the one-step translation along the chain. The Hamiltonian $H_{j-1,j}$ is invariant under this operation: $(U_j(\phi)T)^\dagger H_{j-1,j}(\phi)(U_j(\phi)T) = H_{j-1,j}(\phi)$. The other is the spin flip operation F defined by $FS_j^z F = -S_j^z$ and $FS_j^\pm F = S_j^\mp$ for any j. The Hamiltonian has this symmetry if and only if $\phi = 0$ or π, i.e., $FH_{j-1,j}(\phi = 0/\pi)F = H_{j-1,j}$. At $\phi = \pi$, there is a hidden algebraic relation: $\{U_j(\pi)T, F\} = 0$ where $\{,\}$ denotes the anticommutator. This can be shown by the fact that $FU_j(\pi)F = U_j(\pi)e^{2\pi i S_j^z} = -U_j(\pi)$ since we consider the half-odd-integer spin chains. From the anticommutation relation, there exist at least two ground states labeled by the quantum number associated to F at $\phi = \pi$. We call two of them $|G(\pi, +1)\rangle$ and $|G(\pi, -1)\rangle \equiv (U_j(\pi)T)|G(\pi, +1)\rangle$, where $F|G(\pi, \eta)\rangle = \eta|G(\pi, \eta)\rangle$. This degeneracy is not restricted to the ground state. From our argument, it is obvious that every energy level is at least doubly degenerate at $\phi = \pi$ and can be distinguished by the eigenvalue of F. An extension to the above argument to other systems with translational symmetry can be done in a straightforward way by replacing $U_j(\phi)T$ with $U_\mathcal{A}(\phi)T_\mathcal{A}$, where $U_\mathcal{A}(\phi) = \prod_{j\in\mathcal{A}} U_j(\phi)$ and $T_\mathcal{A}$ is the translation of the unit layer.

To discuss the relation between this degeneracy and the LSM theorem, it is useful to introduce the translationally invariant Hamiltonian with the twist ϕ as $\tilde{H}(\phi) \equiv U^\dagger(\phi)H_{L,1}(\phi)U(\phi)$, where $U(\phi) = \prod_{j=1}^L U_j(-j\phi/L)$. The level-crossing at $\phi = \pi$ suggests that one of the excited state of $\tilde{H}(0) = H_{L,1}(0)$ is smoothly connected to the ground state of $\tilde{H}(2\pi)$. Since $H_{L,1}(2\pi) = H_{L,1}(0)$, the ground state of $\tilde{H}(2\pi)$ is given by $U^\dagger(2\pi)|G(0)\rangle$, where $|G(0)\rangle$ is the ground state of $\tilde{H}(0)$. Finally, along the same lines as the LSM argument, one can show that $U^\dagger(2\pi)|G(0)\rangle$ is orthogonal to $|G(0)\rangle$ and the energy difference between them is $\mathcal{O}(1/L)$ using the translational and F symmetry.

Another comment is that, in the case of one dimensional spin chains with open boundary condition, the local gauge twists are always gauged away. Using the gauge transformation of the string type, $\prod_{i=1}^j U_i(\phi) = e^{i\sum_{i=1}^j (S-S_i^z)\phi}$, we obtain the Berry phase as $\gamma_{j,j+1} = 2\sum_{i=1}^j S_i\pi$ assuming the energy gap. It is consistent with the generic VBS state [21]. As for the $S = 1$ spin chain with open boundaries, the Haldane gap corresponds to the energy gap above the Kennedy triplet[13]. Then the Berry phase of the low energy cluster below the Haldane gap, which includes contribution of the edge states, gives vanishing Berry phase. It should be distinguished from the translationally invariant case without edge [19, 25].

Further this present argument is also applicable for systems with charge degrees of freedom. Let us consider a fermion model with conserved particle number $n_{tot} = \sum_i n_i$ such as spinless fermions with interaction $H = \sum_{\langle ij \rangle}(tc_i^\dagger c_j + h.c. + V_{ij}n_i n_j)$, where $n_i = c_i^\dagger c_i$ and c_i is a fermion annihilation operator at site i. The $U(1)$ gauge twist against the charge degree of freedom is introduced by replacing a hopping at the special link (ij) as $e^{i\phi}c_i^\dagger c_j$ and the $U(1)$ local gauge transformation is given by

$$U_j(\phi) = e^{in_j\phi}.$$

Then the transformation property of the Berry phase under the gauge transformation leads the relation

$$\gamma_{\text{In}} = \gamma_{\text{Out}} - 2\pi \sum_{i\in\mathcal{A}} \tilde{n}_i,$$

where $\tilde{n}_i = \frac{1}{2\pi}\int\langle\phi|n_i|\phi\rangle d\phi$ as the case of spins and $\mathcal{A}$ is a unit layer. Following the same argument as the spin case, the translational symmetry gives a requirement for the gap under the twist as

$$\rho \in \mathbb{Z}, \quad \rho = \frac{1}{N}\langle\sum_j n_j\rangle$$

where ρ is an average particle number per unit layer and N is a number of the unit layers. It has also a non-Abelian extension for the degenerate multiplet which is just a repetition of the spin case. It requires that, when the filling is $\rho = p/q$ with mutual co-prime p and q, there exists a multiplet of M states in the low energy spectrum to form a cluster, which is separated from the else under the twist as $M = q\ell$, $\ell = 1, 2, \cdots$, $\rho = p/q$. [27, 32, 33]

Reflection symmetry We may further apply the present argument for the generic symmetry, such as a reflection symmetry. Consistency between the possible

Berry phases and the reflection symmetry of the physical system requires some restriction. Let us consider a reflection symmetric system consisting of two subsystems R and L which are mirror images of one another. We first choose a set of sites $\mathcal{A}$ where we perform a gauge transformation. $\mathcal{A}$ itself is chosen to be reflection symmetric. See FIG.2(a) for the simplest example. Then we define the Berry phase γ_L by twisting some links on the boundary of $\mathcal{A}$: $\partial\mathcal{A}$. Note that the self-reflection-symmetric bond, the mirror image of this bond is itself, is not twisted. We denote this Berry phase as γ_L, and the symmetric partner of γ_L as γ_R. Our gauge transformation of the Berry phase results in $\gamma_L = -\gamma_R + 2\pi \sum_{j\in\mathcal{A}} (S_j - \tilde{m}_j)$. The relations $-\gamma_R \equiv \gamma_R, \mod 2\pi$ and $\tilde{m}_j = 0$ hold if the time reversal symmetry is also present. In such case, we obtain that $\gamma_L = \gamma_R + 2\pi \sum_{\mathcal{A}} S_j$. Since the reflection symmetry of the physical structure implies $\gamma_L \equiv \gamma_R, \mod 2\pi$, when the following case,

$$\sum_{j\in\mathcal{A}} S_j \notin \mathbb{Z},$$

we predicts a level crossing during the twisting. Our argument can be extended without any difficulty for generic reflection symmetric models including even three-dimensional ones. Numerical results showing the pattern of level crossings are given in Fig.2(b). Note that there is the ground state degeneracy at $\phi = \pi$. Similarly to the translational symmetric case, this degeneracy can also be explained by mutually anticommuting symmetry operations $U_{\mathcal{A}}(\pi)R$ and F if there is no magnetic field and $\sum_{j\in\mathcal{A}} S_j \notin \mathbb{Z}$, where R denotes the reflection. Similar arguments can be applied to the molecular magnets with Dzyaloshinsky-Moriya(DM) interactions. We can also apply this argument for the Majumdar-Ghosh model of length $4n + 2$ ($n \in \mathbb{N}$) with a periodic boundary condition [34]. It gives a gap closing under the twist, which is consistent with the doubly degenerate ground state at $\phi = 0$.
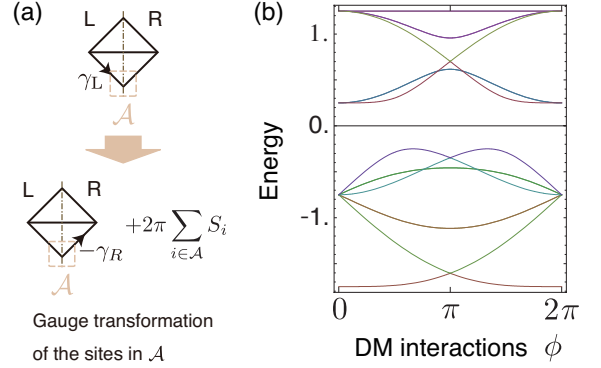
FIG. 2: (a) The definition of the $\mathcal{A}$ in the reflection symmetric system, and the gauge transformation of the Berry phase. The system is reflection symmetric about dashed line. (b) Spectral flow of a reflection symmetric $S = 1/2$ Heisenberg model with DM interactions ϕ. The shape of lattice is the one in (a). At $\phi = \pi$, all states are at least doubly degenerate. Some of them are doubly degenerate for all of the twist ϕ.

* Electronic address: hirano@pothos.t.u-tokyo.ac.jp
† Electronic address: katsura@appi.t.u-tokyo.ac.jp
‡ Corresponding author; Electronic address: hatsugai@sakura.cc.tsukuba.ac.jp

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